TensorNetwork2024 @石川県政記念館しいのき迎賓館, 2024/11/16

Low-rank quantics tensor train representations of Feynman diagrams for multiorbital electron-phonon models

arXiv:2405.06440v3

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Tensor network techniques

Wave function

MPS **DMRG**

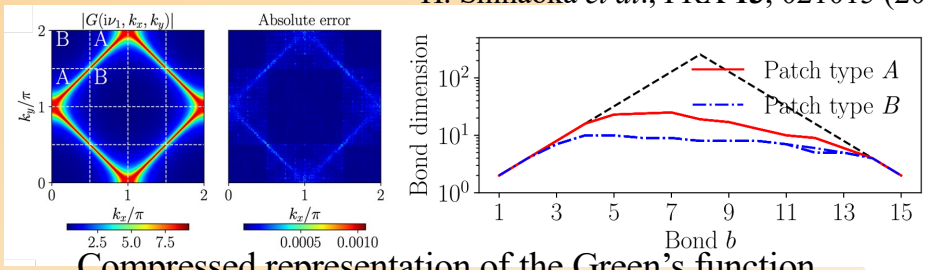
MERA

Application to field theory

- **Data compression**
- **Improved efficiency of operations**

① Quantics Tensor Train (QTT)

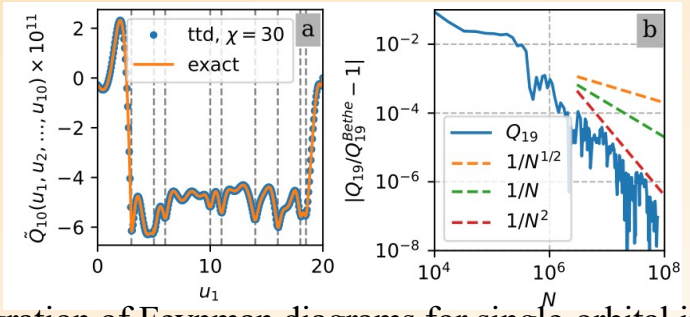
H. Shinaoka *et al.*, PRX **13**, 021015 (2023)



Compressed representation of the Green's function

② Tensor Cross Interpolation (TCI)

Y. N. Fernández *et al.*, PRX **12**, 041018 (2022)



Integration of Feynman diagrams for single-orbital impurity sysmems

Can we solve
strongly correlated electronic systems
by quantum field theory + tensor network?

Method: ① Quantics Tensor Train (QTT)

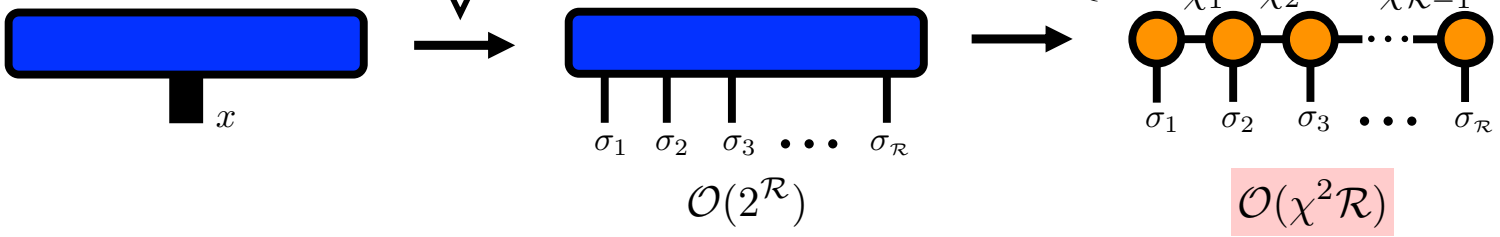
I. V. Oseledets, Dokl. Math. **80**, 653 (2009)
B. N. Khoromskij, Constr. Approx. **34**, 257 (2011)

Quantics representation

Discretization based on binary representation.

$$x \in [0,1) \rightarrow \sum_{r=1}^{\mathcal{R}} \frac{\sigma_r}{2^r} = (0.\sigma_1\sigma_2\cdots\sigma_{\mathcal{R}})_2 = (\sigma_1, \sigma_2, \cdots, \sigma_{\mathcal{R}}) \quad (\sigma_r = 0 \text{ or } 1)$$

Long scale **Short scale**



$\mathcal{O}(2^{\mathcal{R}})$ $\mathcal{O}(\chi^2\mathcal{R})$

Operations in the TT format
- Fourier transforms
- **Integration**

The bond dimension χ_ℓ does not depend on $\mathcal{R}$ (low-rank structure).

→ **Exponential resolution** with linear memory!

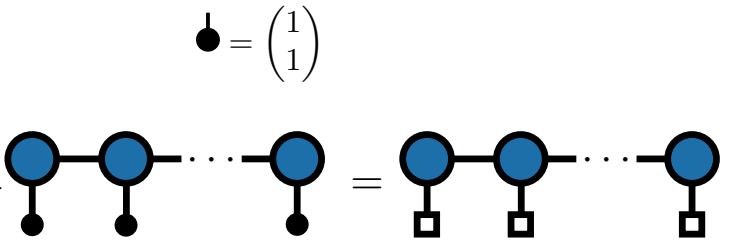
Method: ① Quantics Tensor Train (QTT)

Integration in QTT format

Once the TT representation is constructed, summation and integration can be performed efficiently.

Discretization error (exponentially small).

$$\int_{[0,1]^N} f(\boldsymbol{x}) d^N\boldsymbol{x} \simeq \frac{1}{2^L}\sum_{i=1}^{2^L} f(x_i) \simeq \frac{1}{2^L}\sum_{\sigma_1=1}^{2}\sum_{\sigma_2=1}^{2}\cdots\sum_{\sigma_L=1}^{2}\tilde{F}_{\boldsymbol{\sigma}} =$$



Error when converting to TT.

The computational cost is $\mathcal{O}(\chi^2 L + \chi^3 L)$.

Method: ② Tensor Cross Interpolation (TCI)

Y. N. Fernández *et al.*, PRX **12**, 041018 (2022)

The bottleneck is the high-dimensional integration of the Feynman diagrams.

$$\Sigma(\tau) = \sum_{\eta_1 \cdots \eta_n} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_d \; G_{\eta_1 \cdots \eta_n}(\tau, \tau_1, \cdots, \tau_d)$$

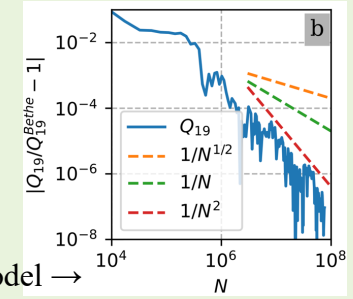
QMC

- **important sampling**
- **convergence** $\sim 1/\sqrt{N}$
- **negative sign problem**

Tensor Cross Interpolation (TCI)

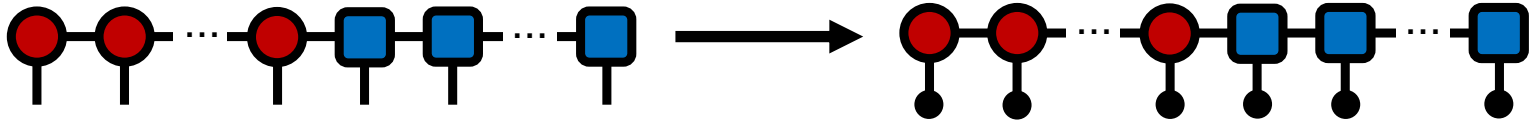
- **local sampling from the state space.**
- **based of low-rank structure**
- **converfence** $\sim 1/N^2$
- **avoid the negative sign problem**

Perturbation expansion of single impurity Anderson model →



Integration using the tensor network

$G_{\eta_1 \cdots \eta_n}(\tau, \tau_1, \cdots, \tau_d) \simeq$

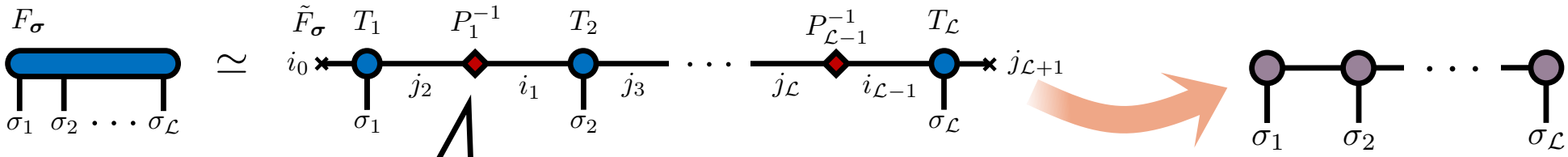


Method: ② Tensor Cross Interpolation (TCI)

Estimating a tensor train by adaptively sampling a function.

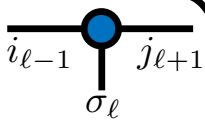
S. Dolgov *et al.*, Comput Phys Commun **246**, 106869 (2020)
Y. N. Fernández,…, H.shinaoka, X.Waintal, arXiv:2407.02454 (2024)

$$F_{\boldsymbol{\sigma}} \simeq \tilde{F}_{\boldsymbol{\sigma}} = [T_1]^{\sigma_1}_{i_0 j_2} [P_1^{-1}]_{j_2 i_1} [T_2]^{\sigma_2}_{i_1 j_3} [P_2^{-1}]_{j_3 i_2} \cdots [P_{\mathcal{L}}^{-1}]_{j_{\mathcal{L}} i_{\mathcal{L}-1}} [T_{\mathcal{L}}]^{\sigma_{\mathcal{L}}}_{i_{\mathcal{L}-1} j_{\mathcal{L}+1}}$$

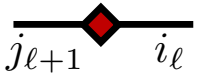


TT format

$[T_\ell]^{\sigma_\ell}_{i_{\ell-1} j_{\ell+1}} = F_{i_{\ell-1} \oplus \sigma_\ell \oplus j_{\ell+1}} =$



$[P_\ell]_{j_{\ell+1} i_\ell} = F_{i_\ell \oplus j_{\ell+1}} =$



$i_\ell \in \mathcal{I}_\ell,\ j_\ell \in \mathcal{J}_\ell$ (subset)

Iterative **local update**
of the pivot list $\{\mathcal{I}_\ell, \mathcal{J}_\ell | \ell = 1, \cdots, \mathcal{L}-1\}$

⚠ Ergodicity problem

Local updates can miss important features.

Today's topic

Previous studies focus on single-orbital Anderson impurity model. → What about multi-orbital systems required for real materials?

Main question

- Does a multi-degree-of-freedom system have a low-rank structure?
- How can we avoid the ergodicity problem in multi-degree-of-freedom systems?

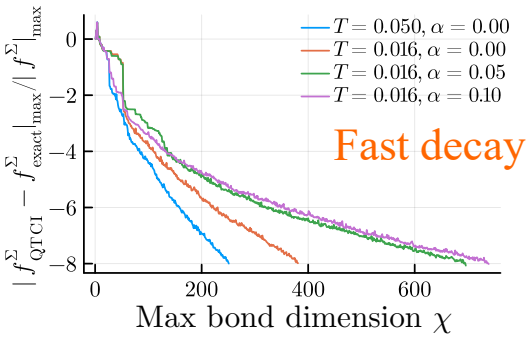
Low-rank structure of Feynman diagrams in a multi-orbital electron-phonon model!

Estimate TT using Quantics TCI

with { **Local updates** / **Global updates** NEW }

$$\Sigma^{(2)}_{\gamma\gamma'}(\tau) = \sum_{\substack{\eta_1 \sim \eta_4 \\ \tau', \tau''}} \gamma' \; \eta_1 \; \eta_2 \; \eta_3 \; \eta_4 \; \gamma \quad (0, \tau', \tau'', \tau)$$

$$\| \quad \gamma \; \gamma' \; \eta_1 \sim \eta_4 \; \tau_1 \; \tau_1' \; \tau_1'' \; \cdots \; \tau_R \; \tau_R' \; \tau_R''$$



Model : Self-energy

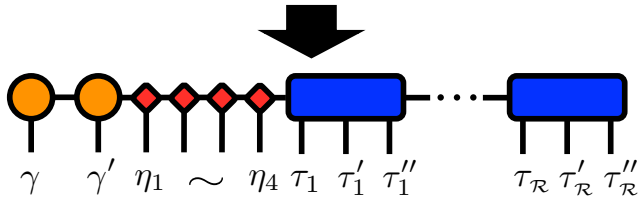
Self-energy for electrons

$$\check{\Sigma}^{(1)}(\tau) = -\sum_{\eta_1\eta_2} g_0^2 D_{\eta_1\eta_2}(\tau)\check{\lambda}^{\eta_1}\check{G}(\tau)\check{\lambda}^{\eta_2}$$

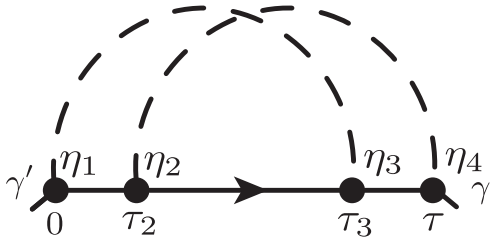
$$\check{\Sigma}^{(2)}(\tau) = \int_{[0,\beta]^2} d\tau' d\tau'' \sum_{\eta_1\eta_2\eta_3\eta_4} g_0^4 D_{\eta_1\eta_3}(-\tau'')D_{\eta_2\eta_4}(\tau'-\tau)$$
$$\times \check{\lambda}^{\eta_4}\check{G}(\tau-\tau'')\check{\lambda}^{\eta_3}\check{G}(\tau''-\tau')\check{\lambda}^{\eta_2}\check{G}(\tau')\check{\lambda}^{\eta_1}$$

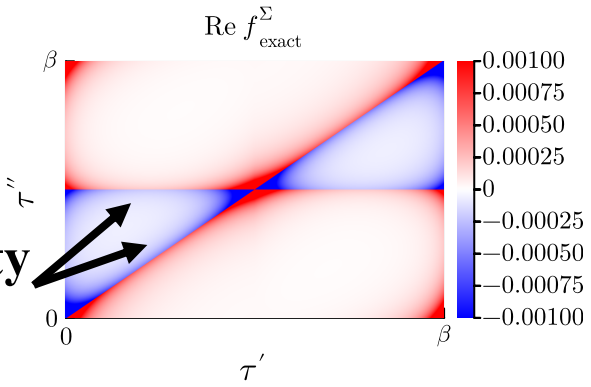
$$\equiv f^{\Sigma}(\gamma,\gamma',\eta_1,\eta_2,\eta_3,\eta_4,\tau,\tau',\tau'')$$

(12, 6, $\mathcal{O}(\beta)$)



First-order calculations are done without using the tensor network.





Discontinuity

Fine feature

The bond dimension is suggested not to diverge at low temperatures. H. Takahashi *et al.*, arXiv:2403.09161

Model : Multi-orbital electron-phonon model

Multi-orbital electron-phonon model Y. Kaga *et al.*, PRB **21**, 214516 (2022)

$$\mathscr{H} = \sum_{ij}\sum_{\gamma\gamma'\sigma}\left(t_{ij}^{\gamma\gamma'} - \mu\delta_{ij}\delta_{\gamma\gamma'}\right)c_{i\gamma\sigma}^{\dagger}c_{j\gamma'\sigma} + \sum_{i\eta}\omega_{\eta}a_{i\eta}^{\dagger}a_{i\eta} + \sum_{i\eta}g_{\eta}(a_{i\eta}+a_{i\eta}^{\dagger})\sum_{\gamma\gamma'\sigma}c_{i\gamma\sigma}^{\dagger}\lambda_{\gamma\gamma'}^{\eta}c_{i\gamma'\sigma} + \alpha\mathscr{H}_{\mathrm{ex}}$$

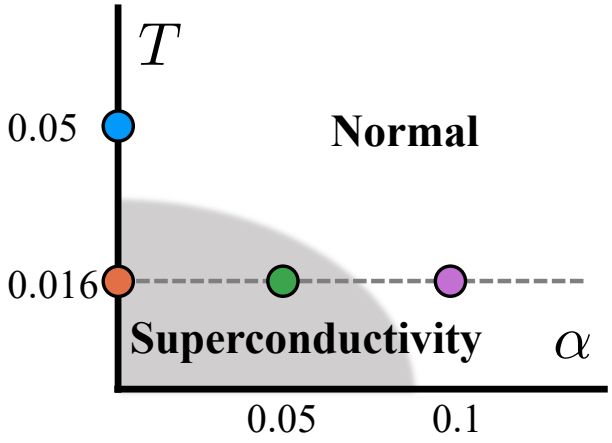
γ, γ' : orbital $(= x, y, z)$
σ, σ' : spin $(=\uparrow, \downarrow)$
η : vibrational mode (6 types)
ω_{η} : phonon energy
g_{η} : electron-phonon coupling
$\alpha\mathscr{H}_{\mathrm{ex}}$: external field of strength α

Local Green's function of electrons

$$\check{G}_{\gamma\sigma,\gamma'\sigma'}(\tau) = -\left\langle \mathcal{T}_{\tau}\Psi(\tau)\Psi^{\dagger}(0)\right\rangle$$

$$\Psi(\tau) = (c_{x\uparrow}(\tau), c_{x\downarrow}(\tau), \cdots, c_{z\downarrow}(\tau), c_{x\uparrow}^{\dagger}(\tau), \cdots, c_{z\downarrow}^{\dagger}(\tau))^{\top}$$

3 orbitals × 2 spins × 2 Nambu components
= **12 flavors**



Result : High-speed error convergence

The interpolation error decreases exponentially regardless of the α and T!

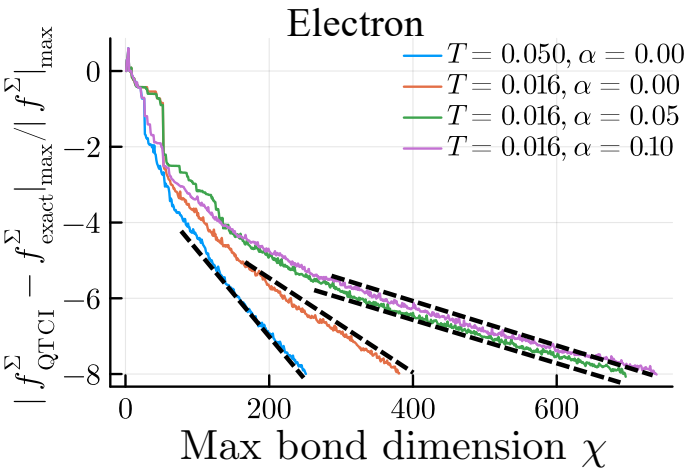
Convergence

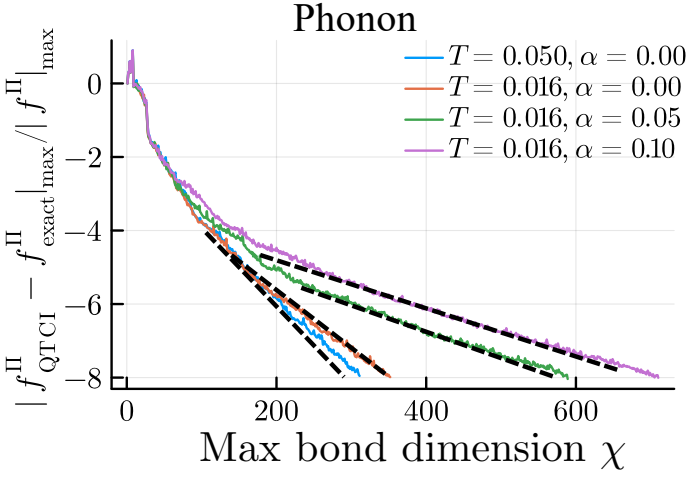
- ✓ Quantum Monte Carlo $(1/\sqrt{N})$
- ✓ TCI (without Quantics, $1/N^2$).

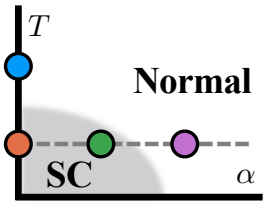
$$\text{Quantics TCI} \propto e^{-\sqrt{N}}$$

N : Number of sampling points

$N \propto \chi^2$

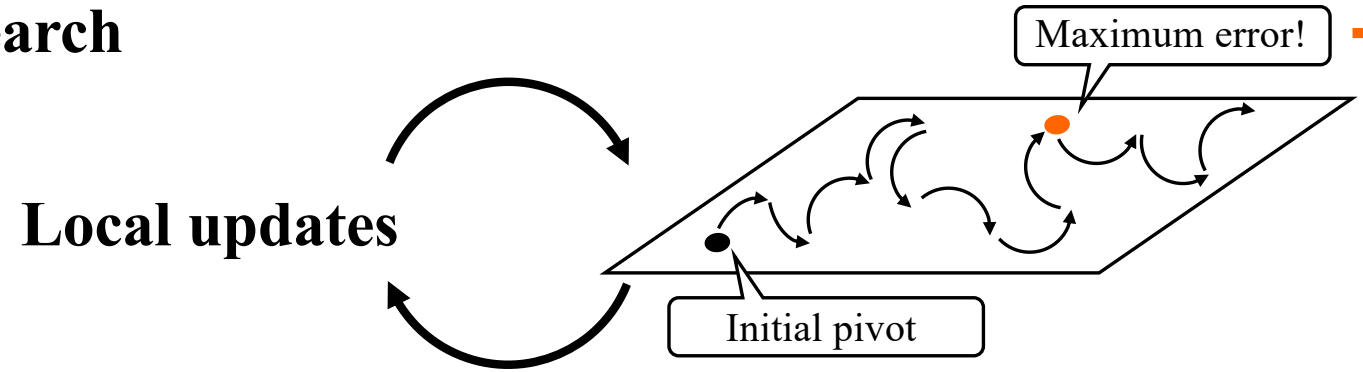






Result : Local updates vs Global updates

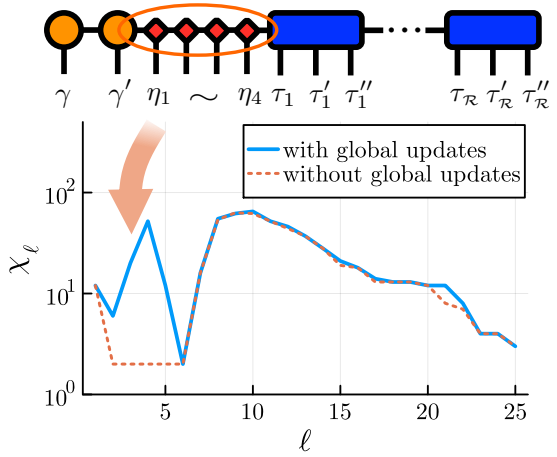
Global search



Local updates miss some sectors of phonons.

⇩

Global updates improve **stability** and **accuracy**.



Summary and Outlook

Summary

1. **Regardless of the magnitude of the external field, both the electron and phonon self-energies have low-rank structures.**
2. **We can avoid the ergodicity problem by combining the local and the global updates**

Outlook

1. **Investigation of the low-rank structure in higher-order Feynman diagrams with/without QTT.**
2. **Replace the quantum Monte Carlo with QuanticsTCI.**

arXiv:2405.06440v3